

Grid Engine for users

Usage & productivity focus

Learning curve ahead...

- Grid Engine has a small number of command-line programs
- Most are very powerful and can be invoked in bewilderingly complex ways
 - Resource requests
 - Job arrays & dependencies
- Man pages and wikis.sun.com will be essential as you get up to speed

Exercise 01

- Goals
 - See Grid Engine in action
 - Run a few commands

Exercise 02

- Goals
 - Submitting, monitoring and naming a few batch jobs
 - The most basic job script ('sleeper.sh')

Exercise 03 - qrsh

- Goals
 - Run real jobs
 - "Instant" Execution via 'qrsh'

qrsh/sqrsh - Reminder

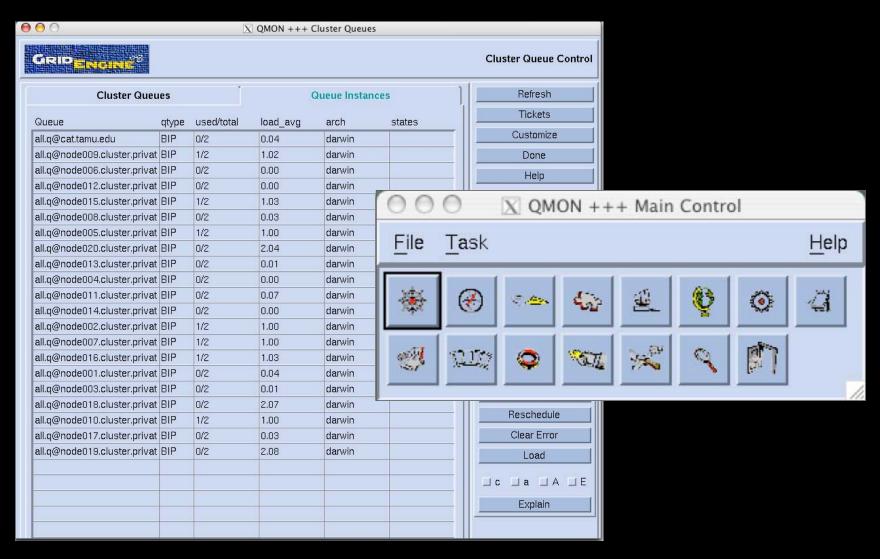
- The Grid Engine 'qrsh' program will run your command or job ASAP on the least loaded node in the system. This is a quick and lightweight way to run short jobs or even test grid engine functionality.
- Note that 'qrsh' commands will fail on clusters where there are no free job slots. These and other error conditions need to be checked for whenever 'qrsh' is used as part of a script or automated workflow.
- Use with some caution be careful of big or resource intensive jobs

Exercise 04

- Goals
 - First intro to job dependencies
 - Trivial chaining
 - Simple binary wrapping for trivial SGE integration
 - Synchronous job submission

Summarizing basic usage

Summarizing basic usage



Most useful SGE commands

- qsub / qdel
 - Submit jobs & delete jobs
- qstat & qhost
 - Status info for queues, hosts and jobs
- qacct
 - Summary info and reports on completed job
- qrsh
 - Get an interactive shell on a cluster node
 - Quickly run a command on a remote host
- qmon
 - Launch the X11 GUI interface

SGE Commands: 'qstat'

cat:~ administrator\$ qstat

job-ID	prior	name	user	state	submit/start	at	queue	slots	ja-task-ID
6	0.56000	first.sh	m010798	r	12/07/2004 10	:13:34	all.q@node002	1	
3	0.56000	first.sh	m010798	r	12/07/2004 10	:04:01	all.q@node005	1	
16	0.56000	hs	sga6043	r	12/07/2004 12	:14:51	all.q@node007	1	
1	0.56000	gr.sh	m010798	r	12/07/2004 09	:47:40	all.q@node009	1	
2	0.56000	first.sh	m010798	r	12/07/2004 10	:01:01	all.q@node010	1	
5	0.56000	first.sh	m010798	r	12/07/2004 10	:11:49	all.q@node015	1	
4	0.56000	first.sh	m010798	r	12/07/2004 10	:08:18	all.q@node016	1	

SGE Commands: 'qstat -f'

cat:~ administrator\$ qstat -f

queuename	qtype	used/tot.	load_avg	arch	states
all.q@cat.tamu.edu	BIP	0/2	0.02	darwin	
all.q@node001.cluster.private	BIP	0/2	0.03	darwin	
all.q@node002.cluster.private 6 0.56000 first.sh m010		1/2 r	1.00 12/07/2004	darwin 4 10:13:34	1
all.q@node003.cluster.private	BIP	0/2	0.00	darwin	
all.q@node004.cluster.private	BIP	0/2	0.01	darwin	
all.q@node005.cluster.private 3 0.56000 first.sh m010		1/2 r	1.00 12/07/2004	darwin 1 10:04:01	1

SGE Commands: 'qhost'

cat:~ administrator	\$ qhost						
HOSTNAME	ARCH	NCPU	LOAD	MEMTOT	MEMUSE	SWAPTO	SWAPUS
global	-	_	_	_	_	_	_
cat	darwin	2	0.03	2.0G	1.4G	0.0	0.0
node001	darwin	2	0.02	2.0G	227.0M	0.0	0.0
node002	darwin	2	1.00	2.0G	274.0M	0.0	0.0
node003	darwin	2	0.00	2.0G	273.0M	0.0	0.0
node004	darwin	2	0.02	2.0G	275.0M	0.0	0.0
node005	darwin	2	1.00	2.0G	274.0M	0.0	0.0
node006	darwin	2	0.02	2.0G	274.0M	0.0	0.0
node007	darwin	2	1.00	2.0G	326.0M	0.0	0.0
node008	darwin	2	0.00	2.0G	271.0M	0.0	0.0
node009	darwin	2	1.00	2.0G	274.0M	0.0	0.0
node010	darwin	2	1.05	2.0G	275.0M	0.0	0.0

SGE Commands: qsub

- Used to submit job scripts to Grid Engine
 - Usage: qsub [options] [scriptfile] [script args]
- qsub finally accepts binaries
 - qsub -b y /bin/hostname
- Powerful
 - 'man qsub' is your friend
 - qsub usage can be as simple or as complicated as you need

Example options

- -A account string; used to group accounting info
- -hold_jid job_id; holds submitted job on job_id
- -l resource=value; requests a specific resource
- -t n[-m[:s]]; array job
- -v, -V; export some or all of your ENV variables

qsub

General format:

```
$ qsub <qsub options> program options>
```

The simplest possible SGE submit syntax would be of this form:

\$ qsub ./myjob.sh

Example: sleeper.sh

```
#!/bin/sh
# Usage: sleeper.sh [time]]
         default for time is 60 seconds
# -- our name ---
#$ -N Sleeper
#$ -S /bin/sh
/bin/echo I am running on host `hostname`.
/bin/echo Sleeping now at: `date`
time=60
if [ $# -ge 1 ]; then
   time=$1
fi
sleep $time
echo Now it is: `date`
```

SGE embedded in jobscripts

```
#!/bin/sh
# Usage: sleeper.sh [time]]
         default for time is 60 seconds
# -- SGE ARGUMENTS --
#$ -N Sleeper
#$ -S /bin/sh
/bin/echo I am running on host `hostname`.
/bin/echo Sleeping now at: `date`
time=60
if [ $# -ge 1 ]; then
   time=$1
fi
sleep $time
echo Now it is: `date`
```

Real world example

```
#!/bin/sh
# Batch-submission script for SGE (Sun GridEngine)
system
# Do we need to re-source our grid engine environment?
source /common/sqe/default/common/settings.sh
## -- Chris Dagdigian; BioTeam Inc.
## -- Embedded grid engine directives follow
#$ -N %NAME%
#$ -o %DIR%/.%JOBID%.qlog.out
#$ -e %DIR%/.%JOBID%.qlog.err
#$ -P glide
#$ -hard -1 glideL-impact-main=1
#$ -hard -1 glideL-impact-glide=4
## -- ok back to work (Glide stuff below) ...
                                                chris@bioteam.net
```

More useful 'qsub' arguments

- All of these can be embedded in scripts, passed via the commandline or passed via the GUI job submission tool
- '-A [string]'
 - Pass a string that will end up in accounting log. Useful for post processing or grouping jobs for grouping and reporting
- '-m b' or '-m e'
 - Mail submitter when job begins/ends
- <u>'-m a' or '-m s'</u>
 - Mail submitter when aborted or suspended
- '-m n'
 - Override all other mail options; Don't send email for any reason

Jobs: Binaries vs. Scripts

- SGE 6 at the CLI assumes scripts
 - "qsub -b y ..." to override
- SGE 6 DRMAA assumes binaries
- 2 main differences in handling
 - For scripts, SGE transfers entire file
 - For binaries, SGE just sends the path

Using Resources

- Resources can be collected together using arithmetic and Boolean operators to form very complex resource requirement strings.
- qsub -hard -l \ arch=solaris64,h_mem_free=800M,swap_free=50M
 ./myJob.sh
 - Job must run on a 64 bit Solaris box with at least 800 MB of free memory and 50 MB of available swap space

Remember:

- You can embed these requests in your scripts so they don't have to be typed all the time
- Can also define "default request" files on a per-user or global level

Default / Preference Files

- Default (qsub) submission settings
 - \$SGE_ROOT/\$SGE_CELL/common/sge_request
 - \$HOME/.sge request
 - \$PWD/.sge_request
- Default (qstat) monitoring settings
 - \$SGE_ROOT/\$SGE_CELL/common/sge_qstat
 - \$HOME/.sge qstat
- Overridden by runtime argments
 - Explicit: "qsub -clear ... "

Monitoring our job with 'qstat'

cat:~ administrator\$ qstat

job-ID	prior	name	user	state	submit/start at	queue	slots ja-task-ID
6	0.56000	first.sh	m010798	r	12/07/2004 10:13:34	all.q@node002	<u>2</u> 1
3	0.56000	first.sh	m010798	r	12/07/2004 10:04:01	all.q@node00!	5 1
16	0.56000	hs	sga6043	r	12/07/2004 12:14:51	all.q@node00	<u>7</u> 1
1	0.56000	gr.sh	m010798	r	12/07/2004 09:47:40	all.q@node009	9 1
2	0.56000	first.sh	m010798	r	12/07/2004 10:01:01	all.q@node010	0 1
5	0.56000	first.sh	m010798	r	12/07/2004 10:11:49	all.q@node01	<u>5</u> 1
4	0.56000	first.sh	m010798	r	12/07/2004 10:08:18	all.g@node010	6 1

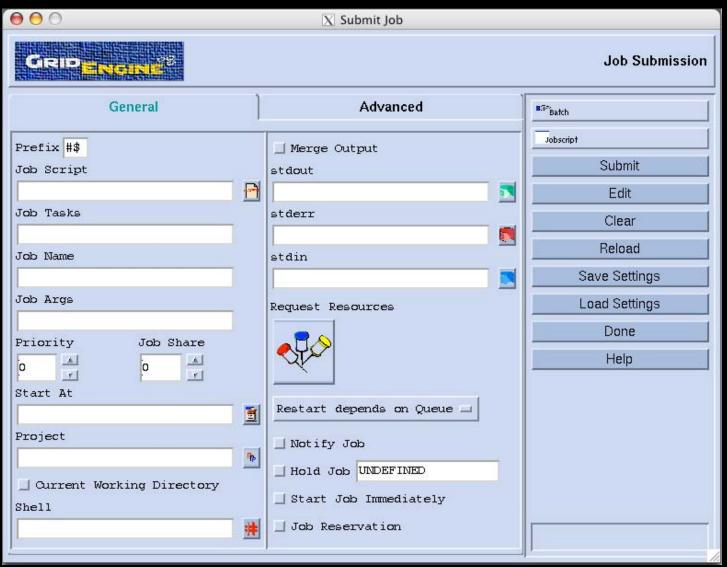
Accounting data with 'qacct'

```
cat:~/sqe-test administrator$ qacct -j 30
_____
           all.q
qname
           node003.cluster.private
hostname
           UNKNOWN
group
           administrator
owner
project
           NONE
department
           defaultdepartment
jobname
           hostname
jobnumber
           30
           undefined
taskid
account
           sqe
priority
qsub time
           Wed Dec 8 09:33:20 2004
start time
           Wed Dec 8 09:42:05 2004
end time
           Wed Dec 8 09:42:05 2004
granted pe
           NONE
slots
failed
exit status 0
ru wallclock 0
```

Via the 'qmon' GUI



Submitting via the GUI



Submitting jobs

- Jobs are submitted via the 'qsub' command
- Many factors affect how/when a job gets dispatched for execution
 - Job resource requirements
 - Availability of eligible execution hosts
 - Various job slot limits
 - Job dependency conditions
 - Fairshare or priority constraints
 - Load conditions

Submitting Jobs

 Important to note that jobs are not necessarily dispatched in the order received

Checking running or pending jobs

We use 'qstat'

Checking completed jobs

```
cat:~/sge-test administrator$ gacct -j 31
             all.q
qname
             node006.cluster.private
hostname
             UNKNOWN
group
owner
             administrator
project
             NONE
department
             defaultdepartment
jobname
             simple.sh
jobnumber
             30
             undefined
taskid
account
             sge
priority
qsub time
             Wed Dec 8 09:33:20 2004
start time
             Wed Dec 8 09:42:05 2004
end time
             Wed Dec
                      8 09:42:05 2004
granted pe
             NONE
slots
failed
             0
exit status 0
ru wallclock 0
```

Job Status Checking: Summary

- For running or pending jobs:
 - Use the 'qstat' command

- For completed jobs:
 - Use the 'qacct' command

About System & Cluster Status

- 'qstat -f'
 - Look for queues in alarm ('a') or ('au') state
 - Look for load averages of 99.99 percent
- 'qhost'

Pending Jobs

- A Jobs initial state when it is submitted to SGE is PENDING.
 - Reported by 'qstat' as state ('qw')
 - (queued waiting)
- Reasons for job remaining in a pending state.
 - No free job slots
 - All queues have hit suspend or load thresholds
 - You have requested an impossible resource

qstat simple usage

- qstat -help
 - More usage info
- qstat
 - Displays current jobs in the system
- qstat -j [job ID or joblist]
 - Shows config and scheduler info for job
- qstat -l [resource string]
 - Shows jobs/queues that provide/need the resource
- qstat -u <user>
 - Show only jobs from that user
- qstat -t
 - Information on array jobs

qstat simple usage continued

- qstat -q [queue]
 - Show jobs running in queue
- qstat -explain
 - More info about the reason queue(s) in alarm state
- qstat -f
 - Full queue summary
- qstat -f -ne
 - Queue summary with empty queues ignored

Possible job states reported by qstat

- 't' -- Transferring
- 'r' -- Running
- 'R' -- Restarted
- 's' -- Suspended
- 'S' -- Suspended by the queue
- 'T' -- Suspend queue threshold reached
- 'w' -- Waiting
- 'h' -- Hold
- 'e' -- Error

Possible queue states reported by qstat

- 'u' -- Unknown (sge_execd or server down?)
- 'a' -- Alarm (load threshold reached)
- 'A' -- Alarm (suspend threshold reached)
- 's' -- Suspended (by user or admin)
- 'd' -- Disabled (by user or admin)
- 'C' -- Suspended (by calendar)
- 'D' -- Disabled (by calendar)
- 'S' -- Suspended (by subordination)
- 'E' -- Error (sge_execd can't reach shepherd)

Demo Time (#5, #6) Array Jobs Simple Workflow

05 - Array Jobs Demo

- Goal
 - See Array Jobs in action
 - Understand them (!)
 - A huge benefit for some types of workflows

06 - Simple Workflow Demo

Goal

 See a simple workflow script that uses arrays and job dependencies to perform a powerful multi-step task

Contrived Use case:

- A 10 element array job representing real scientific "work"
- A post processing job that is dependent on completion of the "work"
- A cleanup script that is dependent on the postprocessing step

Questions?

Debugging SGE problems

Debugging SGE Problems

- When you:
 - Can't run SGE commands
 - Command not found
 - System not responding
 - Remote operation permission denied
- Try:
 - qhost and 'qstat -f'

- Job level problems
 - Run:
 - qsub -w v <full job request>
- This will tell you if the job can run if
 - All slots on all queues were empty
 - All load values were ignored
- Good source of info on 'why can't my job be scheduled' problems

- Job level problems with pending jobs
 - Run:
 - qstat -j <job_id>
- This will tell you why the job is pending and if there are any reasons why queues cannot accept the job

- Many times the problems are not SGE related
 - Permission, path or ENV problems
- Best thing to do is watch your STDERR and STDOUT
 - Use the qsub '-e' and '-o' switches to send output to a file that you can read
 - Use qsub '-eo' to send STDOUT and STDERR to the same file (useful for debugging)

- To get email listing why a job aborted
 - Use: 'qsub -m a <u>user@host</u> [rest of command] '

- Checking exit status and seeing if jobs ran to completion without error
 - Use: 'qacct -j <job_id>' to query the accounting data
 - Will also tell you if the job had to be requeued onto a different queue or exechost

Final word on debugging ...

- SGE Admins have many more tools
 - Scheduler trace/profile/monitoring
 - Jobdir "keep_active=true"
 - SGE debug ENV variables
- Tip:
 - Ask for help if you get stuck

More Grid Engine Usage

Jobs pending on resources...

[sgeadmin@portal examples]\$ qstat								
job-ID	prior	name	user	state	submit/star	ct at	queue	master
72	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfal.q	MASTER
71	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa10.q	MASTER
67	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa2.q	MASTER
73	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa3.q	MASTER
70	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa4.q	MASTER
69	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa5.q	MASTER
66	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa6.q	MASTER
68	0	Sleeper	sgeadmin	r	12/20/2002	01:00:38	cfa7.q	MASTER
65	0	Sleeper	sgeadmin	r	12/20/2002	01:00:22	cfa8.q	MASTER
64	0	Sleeper	sgeadmin	r	12/20/2002	01:00:22	cfa9.q	MASTER
74	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:26		
75	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:27		
76	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:27		
77	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:28		
78	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:28		
79	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:29		
80	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:29		
81	0	Sleeper	sgeadmin	qw	12/20/2002	01:00:30		
82	0	Sleeper	sgeadmin	qw	12/20/2002			
83		Sleeper	sgeadmin	qw	12/20/2002	01:00:31		

Jobs pending on resources...

```
chrisdag:tmp dag$ gstat -j 46
job number:
exec file:
                            job scripts/46
submission time:
                            Wed Mar 26 10:03:33 2008
owner:
uid:
                            501
group:
                            daq
qid:
                            501
sge o home:
                            /Users/dag
sge o log_name:
                            daq
sge o path:
                            /opt/sqe/bin/darwin-
x86:/usr/local/bin:/usr/local/sbin:/opt/bin:/opt/sbin:/opt/mysql/bin:\
/sw/bin:/sw/sbin:/usr/bin:/bin:/usr/sbin:
sge o shell:
                            /bin/bash
sge o workdir:
                            /private/tmp
sge o host:
                            chrisdag-aliased
account:
                            sqe
cwd:
                            /private/tmp
path aliases:
                            /tmp mnt/ * * /
hard resource list:
                            arch=solaris64
mail list:
                            dag@chrisdag-aliased
notify:
                            FALSE
job name:
                            Sleeper
jobshare:
shell list:
                            /bin/sh
env list:
script file:
                             ./sleeper.sh
scheduling info:
                            queue instance "test.q@chrisdag-aliased" dropped because it is disabled
                            (-1 arch=solaris64) cannot run at host "chrisdag-aliased" because it offers only
hl:arch=darwin-x86
```

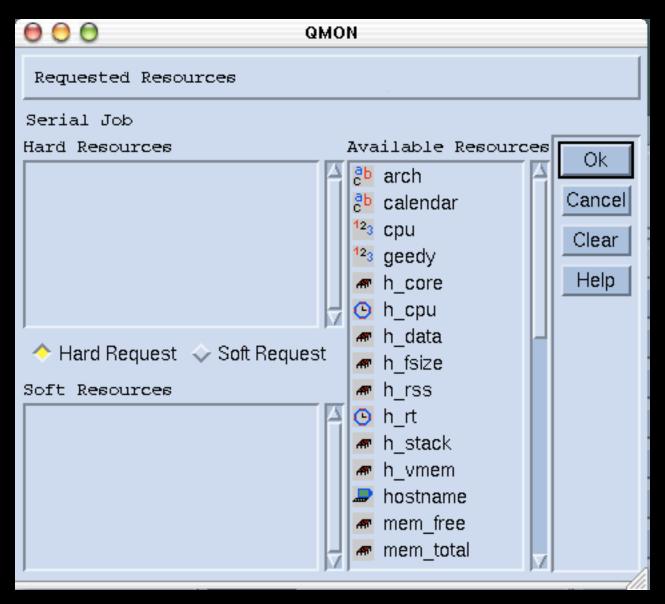
Using Resources

- Resources can be collected together using arithmetic and Boolean operators to form very complex resource requirement strings.
- qsub -hard -l \ arch=solaris64,h_mem_free=800M,swap_free=50M
 ./myJob.sh
 - Job must run on a 64 bit Solaris box with at least 800 MB of free memory and 50 MB of available swap space

Remember:

- You can embed these requests in your scripts so they don't have to be typed all the time
- Can also define "default request" files on a per-user or global level

Available default resources



Queue instance resources

```
cat:~/sqe-test administrator$ qconf -se node001.cluster.private
                      node001.cluster.private
hostname
load scaling
                      NONE
complex values
                      NONE
load values
                      np load long=0.000000,load short=0.006836, \
                      load medium=0.019043,load long=0.000000,arch=darwin, \
                      num proc=2,mem free=1820.000000M,swap free=0.000000M, \
                      virtual free=1820.000000M,mem total=2048.000000M, \
                      swap total=0.000000M,virtual total=2048.000000M, \
                      mem used=228.000000M,swap used=0.000000M, \
                      virtual used=228.000000M,cpu=0.600000, \
                      np load avg=0.009522,np load short=0.003418, \
                      np load medium=0.009522,load avg=0.019043
processors
user lists
                      NONE
xuser lists
                      NONE
projects
                      NONE
xprojects
                      NONE
usage scaling
                      NONE
report variables
                      NONE
```

Resources you may care about

- Example: MatLab licenses
- Handled via Grid Engine "System Complex" or "Load Sensor" mechanisms
- A FlexLM license is a special type of "user requestable, consumable resource"

Example: Licensed MatLab Jobs

- You must request the MatLab "resource"
- Assume cluster currently has 3 floating licenses:
- Usage would be:
 - qsub -hard -l matlab=1 ./matlabscript.sh
 - Or embedded inside a script:
 - #\$ -hard -l matlab=1

Exercise: Array Job Example

- Array Jobs are extremely powerful
- Very efficiently handle the problem:
 - "how do I run application X many, many times with only minor changes in the command line arguments?

Exercise: Array Job example

- Why this matters
 - Grid Engine can probably handle a few tens of thousands of standalone jobs at any one time.
 - Grid Engine 6 has a design goal of handling 500,000 element job arrays

Exercise: Array Job example

 Experiment with the array job example script and input data

Lab Time (07_greedyJobs)

"How do I guarantee my job will get sole access to a compute node so it does not have to compete with another running job for resources?"

A few words on Resource Quotas

Resource Quotas

- The main enhancement to SGE 6.1
- Will likely have a significant impact
- Solves multiple issues that have been bothering SGE admins for years:
 - max_u_jobs on a per-host basis
 - Max jobs per user on a per-queue basis
 - Per user slot limits on parallel environments

Why quotas matter to users

- Good & Bad
 - Just another way for management to slow you down right?
 - Well ...
 - Much potential for serious good
 - Very flexible and powerful capabilities
 - Removes the need for nasty hacks and global limis that SGE admins have had to invent over time

Why quotas matter to users

- Key message
 - Another subsystem you should be aware of
 - Like tickets & policies
 - ... so you know what is going on with your jobs and workflow
 - and so you can better communicate with the admins regarding your needs

Resource Quotas

- Syntax similar to firewall rules
- Simple Example
 - "Iimit slot access to user1 and user2 on every host in the @LinuxHosts hostgroup (except for host penguin03)"

```
name example_resource_quota_set
enabled true
limit users {user1,user2} hosts {@LinuxHosts, !penguin03} to slots=1
}
```

Resource Quotas

- Syntax
 - Multiple rule sets contain one or more rules
- First matching rule from each set wins
- Strictest rule set wins
- Rules can contain
 - Wildcard (*)
 - Logical not operator (!)
 - Brackets ({})
 - Means "treat this rule as per-member" instead of as a group

Quota Command Line

- For Admins
 - qconf -[AaMmds]rqs
 - The usual "Add, modify, delete, show" arg modifiers apply
 - Wizard methods work
 - qconf -mattr resource_quota enabled false rule_1
- For Users & Admins
 - New binary "qquota" in 6.1
 - Also honors a ".sge_qquota" preference file
 - \$SGE_ROOT/\$CELL/common/sge_qquota
 - \$HOME/.sge_qquota

 "The total number of running jobs from project "killerApp" should not exceed 40"

```
name project_limit
description Throttle killerApp projects to 40 concurrent
enabled true
limit project killerApp to slots=40
```

"No power user should have more than 10 running jobs"

```
name power_limit
description Limit all power users
enabled true
limit users {@power} to slots=10
}
```

 "Total number of running jobs from power users should not exceed 40, everyone else is limited to max 5 running jobs each"

```
name power_limit
description Limit all power users
enabled true
limit users @power to slots=40
limit users {*} to slots=5
```

"The total number of jobs without projects must not exceed 10"

```
name nonproject_limit
description Limit jobs without project affiliation
enabled true
limit projects !* to slots=10
}
```

Quota checking for users

- New program 'qquota'
- Man page has best usage
- By default:
 - Shows you all in-play quota rules that apply to the calling user

END;

Thanks!